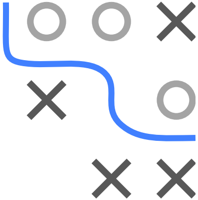
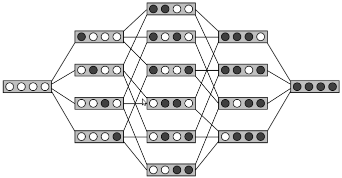
# Introduction to Machine Learning

# Feature Selection: Wrapper methods

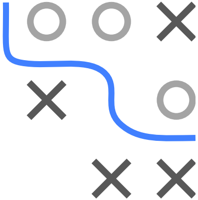




## Learning goals

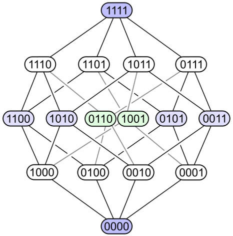
- Understand how wrapper methods work
- Understand how they can help in feature selection
- Know their advantages and disadvantages

# INTRODUCTION



- Wrapper methods emerge from the idea that different sets of features can be optimal for different learners
- Wrapper is a discrete search strategy for $S$, where objective criterion is test error of learner as function of $S$. Criterion can also be calculated on train set, approximating test error (AIC, BIC)

$\Rightarrow$ Use the learner to assess the quality of the feature sets

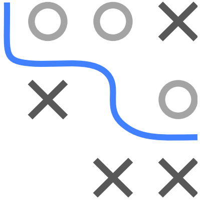



Hasse diagram illustrating search space. Knots are connected if Hamming distance = 1
(Source: Wikipedia)

# OBJECTIVE FUNCTION

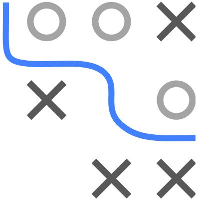
Given $p$ features, **best-subset selection problem** is to find subset $S \subseteq \{1, \dots p\}$ optimizing objective $\Psi : \Omega \to \mathbb{R}$:

$$S^* \in \arg\min_{S \in \Omega}\{\Psi(S)\}$$



- $\Omega$ = search space of all feature subsets $S \subseteq \{1, \dots, p\}$. Usually we encode this by bit vectors, i.e., $\Omega = \{0, 1\}^p$ (1 = feat. selected)
- Objective $\Psi$ can be different functions, e.g., AIC/BIC for LM or cross-validated performance of a learner
- Poses a discrete combinatorial optimization problem over search space of size = $2^p$, i.e., grows exponentially in $p$ (power set)
- Unfortunately can not be solved efficiently in general (NP hard; see, e.g., ▸ Natarajan, 1995)
- Can avoid searching entire space by employing efficient search strategies, traversing search space in a “smart" way

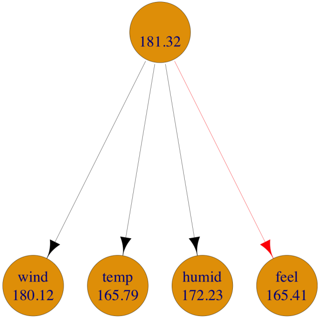
# GREEDY FORWARD SEARCH



Let $S \subset \{1, \ldots, p\}$ be subset of feature indices.

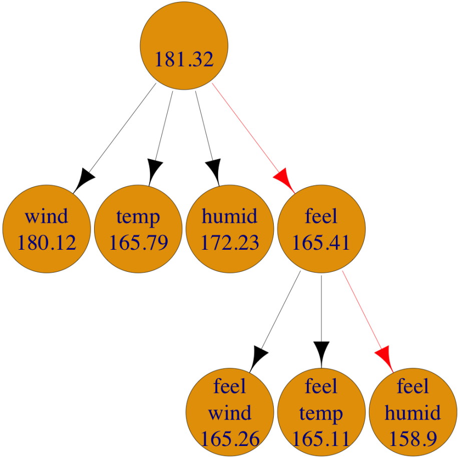
1. Start with the empty feature set $S = \emptyset$
2. For a given set $S$, generate all $S_j = S \cup \{j\}$ with $j \notin S$.
3. Evaluate the classifier on all $S_j$ and use the best $S_j$

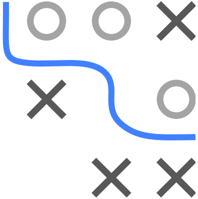
**Example** GFS on a subset of bike sharing data with features windspeed, temp., humidity and feeling temp. Node value is RMSE.



# VISUALIZATION OF GFS

4. Iterate over this procedure



# VISUALIZATION OF GFS

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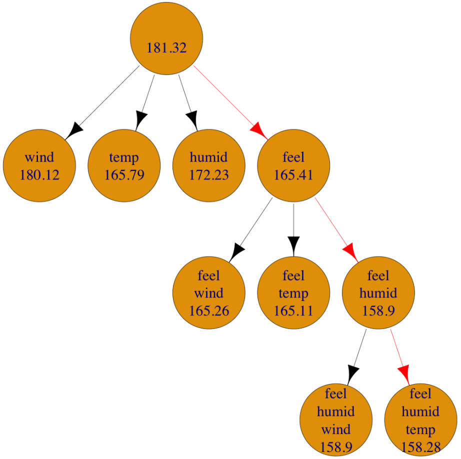


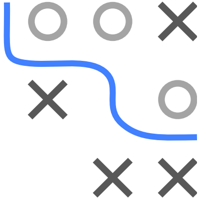

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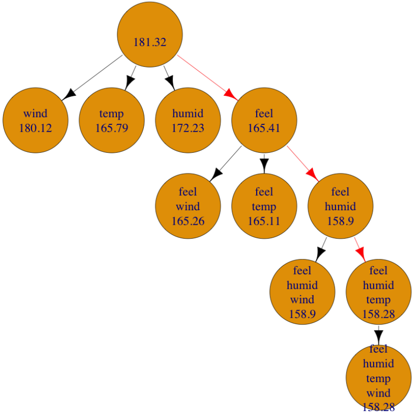
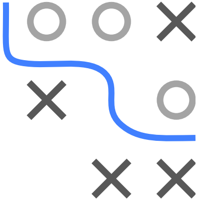


5. Terminate if performance does not improve further or max. number of features is used

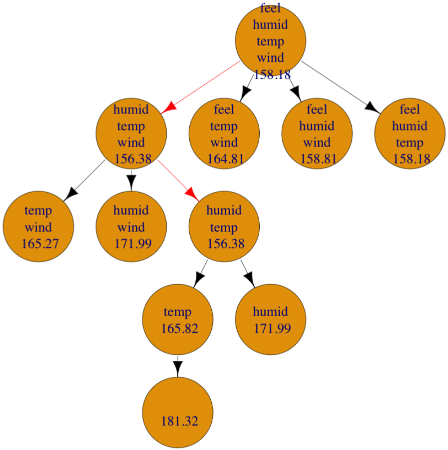
# GREEDY BACKWARD SEARCH

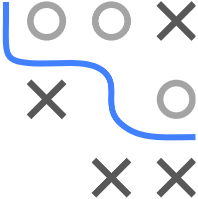
- Start with the full index set of features $S = \{1, \ldots, p\}$.
- For a given set $S$ generate all $S_j = S \setminus \{j\}$ with $j \in S$.
- Evaluate the classifier on all $S_j$ and use the best $S_j$.
- Iterate over this procedure.
- Terminate if:
  - the performance drops drastically, or
  - a given performance value is undershot.

- GFS is much faster and generates sparser feature selections
- GBS much more costly and slower, but sometimes slightly better.

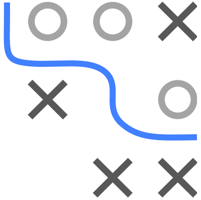
# VISUALIZATION OF GBS

**Example** Greedy Backward Search on bike sharing data



# EXTENSIONS

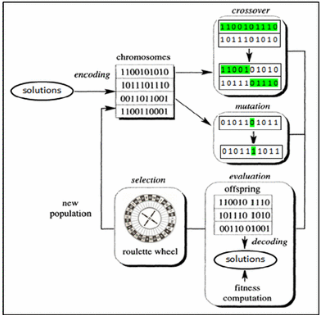


- Eliminate or add multiple features at once to increase speed
- Allow alternating forward and backward search (also known as stepwise model selection by AIC/BIC in statistics)
- Randomly sample candidate feature subsets in each iteration
- Focus search on regions of feature subsets where an improvement is present

# EXTENSIONS: GENETIC ALGORITHMS FOR FS

**Example** Template for $(\mu + \lambda)$-Evolutionary Strategy applied to FS

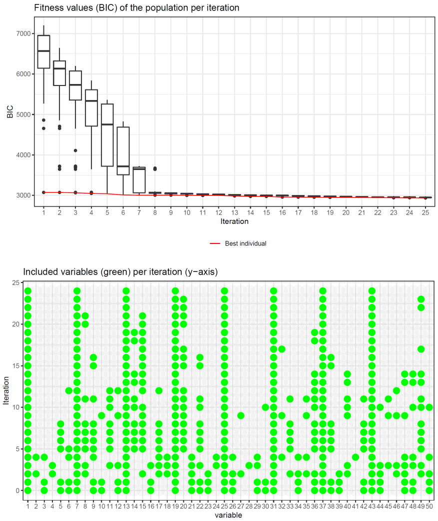
1. Initialization: $\mu$ random bit vectors (feature inclusion/exclusion)
2. Evaluate model performance for bit vectors
3. Select $\mu$ fittest bit vectors (parents)
4. Generate $\lambda$ offspring applying crossover and mutation
5. Select $\mu$ fittest bit vectors from $(\mu + \lambda)$ options for next generation
6. Repeat steps 2-5 until stopping criterion is met




Gu & Cheng, 1996

- Use CV/validation set for evaluation to avoid overfitting
- Choice of $\mu$ and $\lambda$ allows some control over exploration vs. exploitation trade-off
- See our optimization lecture for further information

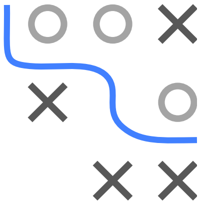
# EXTENSIONS: GENETIC ALGORITHMS FOR FS




**Top**: BIC over number of iterations.

**Bottom**: Bit representation of selected features over iterations.

# WRAPPERS



**Advantages:**

- Can be combined with every learner
- Any performance measure can be used
- Optimizes the desired criterion directly

**Disadvantages:**

- Evaluating target function is expensive
- Does not scale well with number of features
- Does not use additional info about model structure
- Nested resampling becomes necessary